UCSB

Numerical Scouts
Research Talk

Unsupervised Chemical Knowledge Discovery via Koopman Mode Decomposition of Concentration Time Series

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January 30, 2020

Key phrases: Koopman operator, unsupervised learning, reaction network, hydrogen oxidation, combustion chemistry

I will present a novel algorithm for learning reaction networks (and other chemical features) from concentration time series in an unsupervised manner. With this I will give a brief introduction to the chemistry of hydrogen oxidation. Then, using data from thousands of molecular dynamics simulations of hydrogen oxidation, I demonstrate analysis with my algorithm. These simulations are ideal as they do not require prior knowledge of possible mechanisms or intermediates - rather these can be learned. After giving a minimal necessary introduction to Koopman operator theory, I will demonstrate that stoichiometry (coefficients of reaction equations) and kinetics (reaction rates) can be rigorously obtained from Koopman eigenvalues, eigenvectors, and modes. If time permits, I will end with discussing how these mathematical objects can be computed from our data.

Location and Time

Engineering II 2243 ME conference room @ 6pm

Pre-requisites

Linear algebra, differential equations, and calculus at the introductory level

Reference

1. Alaghemandi, Mohammad, Lucas B. Newcomb, and Jason R. Green. "Ignition in an atomistic model of hydrogen oxidation." *The Journal of Physical Chemistry A* 121.8 (2017): 1686-1692.

2. Arbabi, Hassan. *Introduction to Koopman operator theory of dynamical systems.* (2018).

3. Brunton, Bingni W., et al. "Extracting spatial-temporal coherent patterns in large-scale neural recordings using dynamic mode decomposition." *Journal of neuroscience methods* 258 (2016): 1-15.